

Androstan-17-one, 3-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-, (3«alpha»,5«alpha»)-

Other names: 3-«alpha»-tert-butyl dimethylsilyloxy-5-«alpha»-androstan-17-one
3-((tert-Butyl(dimethyl)silyl)oxy)androstan-17-one-, (3alpha,5alpha)-
Androsterone, TBDMSi (3-O)

Androsterone, tert-butyl dimethylsilyl ether

5«ALPHA»-androstan-3«alpha»-ol-17-one, tbdms derivative

Inchi: InChI=1S/C25H44O2Si/c1-23(2,3)28(6,7)27-18-12-14-24(4)17(16-18)8-9-19-20-10-11-22

InchiKey: UGWVQACEZWDYMD-QNCNMWFGSA-N

Formula: C25H44O2Si

SMILES: CC12CCC3C(CCC4CC(O[Si](C)(C)C(C)(C)C)CCC43C)C1CCC2=O

Mol. weight [g/mol]: 404.70

CAS: 57711-45-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.95		Crippen Method
logp	6.989		Crippen Method
rinpol	2702.00		NIST Webbook
rinpol	2740.00		NIST Webbook
rinpol	2788.80		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C57711452&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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